Coherent Imaging: Materials Science

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We are assessing X-ray diffraction microscopy by phase retrieval as a means to perform high-resolution three-dimensional characterisation of non-periodic isolated objects (particles). Several recent experimental and computational developments have enabled us to perform full 3D X-ray diffraction imaging, with high resolution in all three dimensions. These 3D reconstructions were performed from the diffraction data alone. These developments include the Stony Brook diffraction apparatus [1], which allows 3D diffraction datasets to be quickly acquired; the *Shrinkwrap-Hybrid Input Output* phase-retrieval algorithm [2], which allows images to be reconstructed *ab initio* from incomplete diffraction datasets; a fast distributed FFT [3] and reconstruction software implemented on a computer cluster, which allows 1024^3 diffraction datasets to be phased in several hours. We have achieved high-resolution 3D reconstructions of both well-characterized test objects and of mesoporous foams that cannot be otherwise characterized. We find that high resolution imaging of thick objects can only be attained in the context of 3D measurement and reconstruction. Reconstruction from diffraction data acquired over many sample orientations allows one to avoid defocus (depth of field) artifacts as well perform a quantitative measurement of refractive index that is not possible from single-view diffraction data. A recent development is the use of reference points deposited near the object to provide an x-ray hologram. The hologram can be used to rapidly identify the specimen, and help the phase-retrieval algorithm.

Resolution of X-ray diffraction imaging will ultimately be limited by radiation damage. One eventual goal is to surpass damage resolution limits of individual particles by using streams of identical particles, such as protein macromolecules, using flash-imaging by X-ray free-electron lasers (XFELs) [4]. Models show that these methods should allow close to atomic resolution imaging.

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